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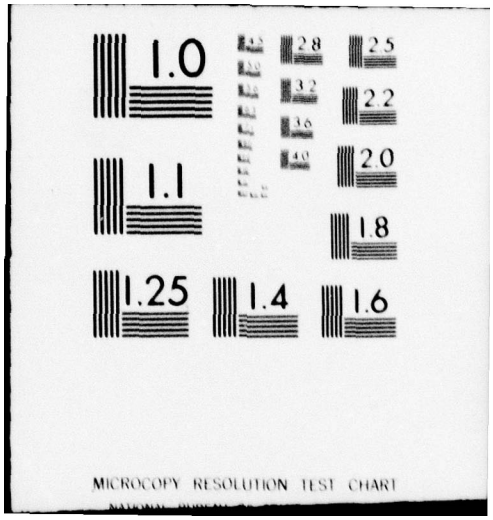
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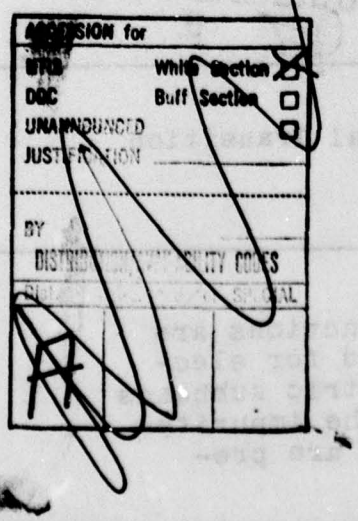
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THEORY OF IMPURITY-SHIFTED INTERSUBBAND TRANSITIONS IN N-TYPE INVERSION LAYERS ON (100) SILICON*

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Binding energies and variational wave functions are calculated as functions of electric field for electron impurity states split off from electric subbands of (100) silicon and silicon dioxide. The impurity-shifted intersubband transition energies are presented.

1. Introduction

The development of MOS devices has stimulated a great deal of interest in the basic properties of inversion layers at semiconductor boundaries. Of some importance are impurities and their associated electronic bound states. We have made a theoretical investigation of several bound states split off from the lowest three electric subbands of an n-type inversion layer on (100) silicon bounded by silicon dioxide.

2. Theoretical Development

We consider two contiguous, semi-infinite half-spaces, one of p-type silicon and the other of silicon dioxide, with a common boundary parallel to a (100) plane of the silicon. We assume that the potential energy of an electron undergoes an infinite discontinuous jump as the electron passes from the silicon into the silicon dioxide. In the region of the inversion layer, there is an electric field which, to a good first approximation[1], can be taken to be constant.

We assume that an impurity ion of charge +Ze is located at the boundary between the silicon and the oxide. For this situation[2], the lowest lying bound states associated with a (100) interface on silicon are derived from the constant energy ellipsoids whose major axes are perpendicular to the interface.

The Hamiltonian is taken to be

$$H = H_o + H_1 \qquad (1)$$

where

$$H_o = -\gamma \frac{\partial^2}{\partial z^2} + \frac{\delta}{z} + \varkappa \mathcal{E} z, \quad z \geq 0 \ , \tag{2}$$

$$H_1 = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + U(\vec{r}) \ , \tag{3}$$

$\gamma = m_t/m_\ell$, $\delta = (\epsilon_2-\epsilon_1)/4Z\epsilon_2$, $\varkappa = \hbar^4(\epsilon_1+\epsilon_2)^3/4Z^3m_t^2e^5$, $\mathcal{E}$ is the electric field in esu, m_t and m_ℓ are the transverse and longitudinal effective masses, and ϵ_1 and ϵ_2 are the dielectric constants of SiO_2 and silicon, respectively. In Eq. (1), energy is measured in units of the effective Rydberg, $Ry^* = 2m_te^4Z^2/\hbar^2(\epsilon_1+\epsilon_2)^2$, and length in units of the effective Bohr radius, $a_o^* = \hbar^2(\epsilon_1+\epsilon_2)/2Zm_te^2$. For the silicon-$SiO_2$ system, $Ry^* = 42.3$ meV and $a_o^* = 21.8$ A. The impurity ion is taken to be at the silicon-SiO_2 interface and screening is neglected, so $U(\vec{r})$ has the Coulomb form

$$U(\vec{r}) = -\frac{2}{|\vec{r}|} \ . \tag{4}$$

The term involving δ in Eq. (2) represents the interaction of the electron with its own image.

In the limit of high electric fields, an adiabatic theorem applies and the impurity wave function has the form

$$\psi(\vec{r}) = \chi_m^{(n)}(x,y) f_n(z) \tag{5}$$

where $f_n(z)$ is an eigenfunction of H_o given by Eq. (2) and corresponds to the electric subband of interest. We consider three subbands and choose the $f_n(z)$ to be variational functions of the Fang-Howard[3] type

$$f_o(z) = A_o z \exp(-\tfrac{1}{2}b_o z) \tag{6a}$$

$$f_1(z) = A_1 z(1-\alpha_1 z)\exp(-\tfrac{1}{2}b_1 z) \tag{6b}$$

$$f_2(z) = A_2 z(1+\alpha_2 z+\beta_2 z^2)\exp(-\tfrac{1}{2}b_2 z) \ . \tag{6c}$$

The quantities b_n are variational parameters, the A_n are normalization constants, and α_1, α_2, and β_2 are chosen so that the functions $f_n(z)$ are orthogonal on the interval $0 \leq z \leq \infty$. We take $\chi_m^{(n)}(x,y)$ to have either of two forms

$$\chi_o^{(n)}(x,y) = B_o \exp[-\tfrac{1}{2}a_o^{(n)}(x^2+y^2)^{\frac{1}{2}}] \tag{7a}$$

$$\chi_{\pm 1}^{(n)}(x,y) = B_1(x \pm iy)\exp[-\tfrac{1}{2} a_1^{(n)}(x^2+y^2)^{\frac{1}{2}}] \qquad (7b)$$

where the B_i are normalization constants and the $a_i^{(n)}$ are variational parameters. The parameters $a_i^{(n)}$ and b_n are varied independently to minimize the expectation value of the Hamiltonian, $\langle H \rangle$. The expectation value of H_o, $\langle H_o \rangle$, is also minimized separately with respect to the b_n to give the continuum energy. The impurity binding energy, E_B, is then given by

$$E_B = \langle H_o \rangle - \langle H \rangle \quad . \qquad (8)$$

3. Results and Discussion

The impurity binding energies have been calculated for electric fields between 10^2 and 10^9 esu for the three lowest subbands and m=0, ±1. The results are plotted in Fig. 1.

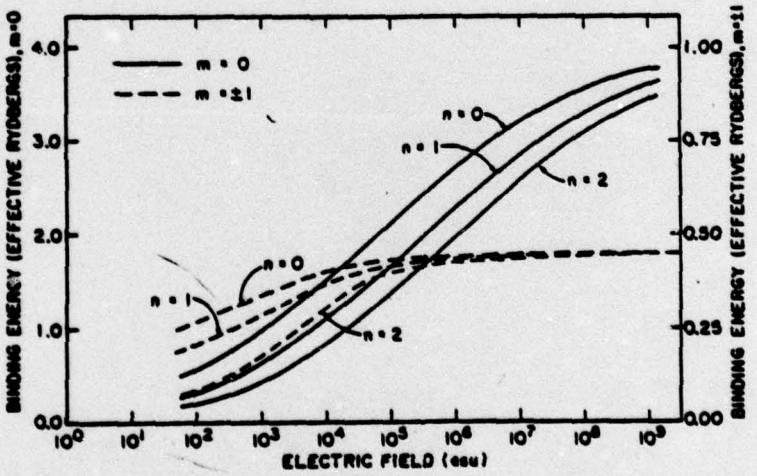

Fig. 1. Impurity state binding energies versus field

The impurity binding energy decreases as one goes from the lowest subband to successively higher subbands for both the m=0 and m=±1 bound states. For a given bound state associated with a given subband, the binding energy increases with increasing electric field and approaches the two-dimensional value in the limit of infinite field.

Electric dipole transitions between subbands are allowed transitions.[3] In Fig. 2 are given our calculated impurity shifted transition energies for the 0→1 and 0→2 inter-

subband transitions when m=0. The transition energies are shifted to higher energies when the electron becomes localized at the impurity. At a field of 10^2 esu, the impurity shifted 0→1 transition is 70 percent higher than the unshifted transition and is only 15 percent lower than the 0→2 unshifted transition. The latter result is in qualitative agreement with recent experimental data.[4] As the electric field increases, the impurity shifted 0-1 transition drops back toward the 0→1 free electron transition and away from the 0→2 free electron transition.

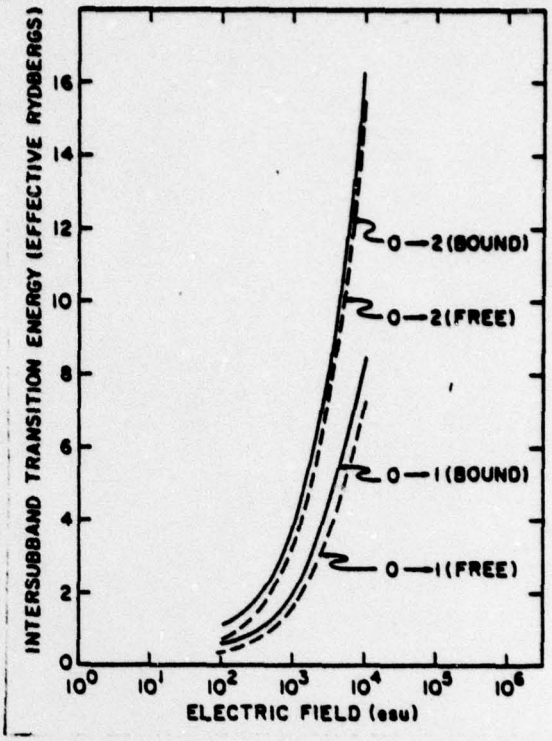

Fig. 2. Intersubband transition energies for bound (m=0) and free states

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